CONTENTS

Molecular structure of furan, determined by combined analyses of data obtained by electron diffraction, rotational spectroscopy and liquid crystal NMR spectroscopy
P.B. Liescheski and D.W.H. Rankin (Edinburgh, Gt. Britain) 1
Determination of the gas-phase molecular structure of tris(trimethylsilyl)(trichlorosilyl)methane by electron diffraction
D.G. Anderson, D.W.H. Rankin and H.E. Robertson (Edinburgh, Gt. Britain), A.H. Cowley and M. Pakulski (Austin, TX, U.S.A.) 21
Mise en évidence par spectrométries optiques de formes tautomères caractéristiques du (bromo-5 pyridyl-2 azo)-2 diéthylamino-5 phenol (bromo PADAP)
T. Delatour el A. Burneau (Vandoeuvre-les-Nancy, France) 31
Infrared spectroscopic investigation of complexes of ClF and Cl_2 with crown ethers and related cyclic polyethers in argon matrices
H. Bai and B.S. Ault (Cincinnati, OH, U.S.A.) 47
Gas-phase structures of perfluorotetraphydrothiophene c-C_4F_8S, tetrahydrothiophene-1-oxide, c-C_4F_8SO, and tetrahydrothiophene-1, 1-dioxide, c-$C_4F_8SO_2$
H.-G. Mack and H. Oberhammer (Tübingen, F.R.G.) and J.M. Shreeve and X.-B. Xia (Mosow, ID, U.S.A.) 57
The conformational equilibrium of $CH_3CH_2CH_2NH_3^+$: Raman study in solution and ab initio calculations
H. Hagemann, H. Bill and J. Mareda (Geneva, Switzerland) 69
Rotational isomerism, structure and vibrational assignment of methoxyallene: joint IR and Raman investigation and non-empirical MO-SCF and valance force field calculations
A. Rastelli and E. Gallinella (Modena, Italy) and M. Burdisso (Pavia, Italy) 79
Torsional transitions and barrier to internal rotation of 1-butyne
G.A. Guirgis and J.R. Durig (Columbia, SC, U.S.A.) and S. Bell (Dundee, Gt. Britain) 101
Reorientational motion of hydroxide ions in solid RbOH and CsOH
J. Henning and M.D. Lutz (Siegen, F.R.G.), H. Jacobs and B. Mach (Dortmund, F.R.G.) 113
Conformational and vibrational analysis of 2-pentyne and 2-hexyne
G.A. Crowder and P. Blankenship (Canyon, TX, U.S.A.) 125
On the correlation between conformational parameters and deformation energies in *syn*-1,6:8,13-diimino[14]annulenes with connected bridges
R. Destro, F. Merati, E. Ortoleva and T. Pilati (Milan, Italy) 133
Molecular structure of cycloheptene, C_7H_{12}, as determined by electron diffraction and molecular mechanics calculations
L.I. Ermolaeva and V.S. Mastryukov (Moscow, U.S.S.R.), N.L. Allinger (Athens, GA, U.S.A.) and A. Almenningen (Oslo, Norway) 151
Crystal structures of the diastereomeric salt pair of the prostaglandin intermediate 1*R*, 2*S*(+)-*cis*-2-hydroxycyclopent-4-enylacetic acid with *S*- and *R*-1-phenylethylamine
M. Czugler and I. Csöregh (Stockholm, Sweden), A. Kálmán, F. Faigl and M. Acs (Budapest, Hungary) 157
Crystal structures of 4,4′-dimethoxydithiophene and comparison with quantum mechanical calculations
E.F. Paulus (Frankfurt, F.R.G.), K. Siam, K. Wolinski and L. Schäfer (Fayetteville, AR, U.S.A.) 171
Electronic structure and conformational properties of the amide linkage. Part 7. Photoelectron spectroscopic and quantum chemical studies of some cyclic ureas and thioureas
G. Irsch and P. Rademacher (Essen, F.R.G.) 181
Electronic absorption spectra of cryogenic systems with hydrogen bonds
T.G. Meister, G.Ya. Zelikina and O.M. Artamonova (Leningrad, U.S.S.R.) 193
An answer to the SPIRO versus ANSA dilemma in cyclophosphazenes. Part XII. the first MEGA-SPIRO and MEGA-ANSA species from trioxodiamines
F. Sournies, A. El Bakili, J.-F. Labarre and B. Perly (Toulouse, France) 201

Crystal and molecular structure of the first MACRO-ANSA and MACRO-SPIRO isomeric cyclophosphazenes $N_3P_3Cl_4$ (HN–$(CH_2)_3$–O–$(CH_2)_2$–O–$(CH_2)_3$-NH)
R. Enjalbert, J. Galy, A. El Bakili, P. Castera, J.-P. Faucher, F. Sournies and J.-F. Labarre (Toulouse, France) 207
Spermine-linked cyclophosphazenes: new DISPIRANSA configurations
G. Guerch, J.-P. Bonnet and J.-F. Labarre (Toulouse, France) 221
An experimental and theoretical study on 2-formyl-and 2,5-diformylfuran
H. Lumbroso and J. Curú (Paris, France), G. Descotes (Villeurbanne, France) and A. Grassi (Catania, Italy) 227
The crystal structure of an incomplete cubane-like trinuclear tungsten cluster $\{[W_3S_4]\cdot[S_2P(OC_2H_5)_2]_3\cdot\mu_2\text{-}CH_3COO\cdot C_5H_5N\}\cdot D.5HCON(CH_3)_2$
H.-Q. Zhan, Y.-F. Zheng, X.-T. Wu and J.-X. Lu (Fujian, People's Republic of China) 241
β-Diketone interactions. Part 9. The X-ray crystal structure of 2,2-difluoro-4,6-dimethyl-5-(4'-nitrophenyl)-1,3,2-dioxaborinane ($C_{11}H_{10}BF_2O_4$)
J. Emsley, N.J. Freeman, P.A. Bates and M.B. Hursthouse (London, Gt. Britain) 249
Conformational structures and torsional potentials in 1,1,2,3-tetrahalogen (F, Cl, Br) propanes
R. Stølevik and P. Bakken (Dragvoll, Norway) 257
Conformational analysis of 4-chlorobutanenitrile and 4-bromobutanenitrile using gas-phase electron diffraction and molecular mechanics calculations
P.J. Stavnebrekk and R. Stølevik (Dragvoll, Norway) 269
Conformational analysis of the halomethyl cyclopropanes and the halosilyl cyclopropanes by molecular mechanics calculations
R. Stølevik and P. Bakken (Dragvoll, Norway) 285
Dynamical aspects of a fast protonic conductor: oxonium perchlorate. Part II. ^1H NMR spin–lattice relaxation
M.H. Herzog-Cance, M. Pham Thi and A. Potier (Montpellier, France) 291
Structural and spectroscopic study of condensed piperidine bicyclanols. 3-Phenethyl-3-azabicyclo[3.2.1.]octan-8-α-ol
E. Galvez, M.S. Arias, I. Ardid, F. Florencio, J. Sanz-Aparicio, J. Bellanato and J.V. Garcia-Ramos (Madrid, Spain) 307
The ^{13}C-NMR chemical shift and the higher order structure of L-alanine residues in tropomyosin in the solid state and in solution
S. Tuzi and I. Ando (Tokyo, Japan) 317
Structural studies of mesogenic orthopalladated imine derivatives
M.A. Ciriano (Zaragoza, Spain), P. Espinet (Valladolid, Spain), E. Lalinde, M.B. Ros and J.L. Serrano (Zaragoza, Spain) 327
Lupin alkaloids. Part II. Some stereochemical aspects of multiflorine and seco(11,12)-12-dehydromultiflorine previously named *N*-methylalbine
T. Brukwicki and W. Wysocka (Poznan, Poland) 343
The electrooptical parameters of aniline and its halogeno derivatives in hydrogen bonded complexes
V.E. Borisenko and A.I. Filarovski (Tyumen, U.S.S.R.) 353

Short communications
The use of constraints in molecular mechanics calculations of medium-sized molecules
A. Beyer, P. Wolschann, A. Becker and G. Buchbauer (Wien, Austria) 371
Electron diffraction study of the molecular structure of tert-butylamine
S. Konaka and N. Yanagihara (Sapporo, Japan) 375

Author Index 383

Subject Index 385